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Es. 1 del 15/1/2018

$$E(\vec{k}) = \underbrace{E_{1s} - \beta}_{\equiv E_0} - 2\gamma(\cos k_x a + \cos k_y a + \cos k_z a)$$

$\Gamma = (000)$ $\quad X = \frac{\pi}{a}(100)$ $\quad M = \frac{\pi}{a}(110)$ $\quad R = \frac{\pi}{a}(111)$

1) Se $\gamma > 0$:

$E(\vec{k})$ max per $(\cos k_x a + \cos k_y a + \cos k_z a) = -3$
cioè $k_x = k_y = k_z = \frac{\pi}{a} \Rightarrow$ **R** (ii)

$E(\vec{k})$ min per $( \ldots ) = +3$
cioè $k_x = k_y = k_z = 0 \Rightarrow$ **Γ** (i)

$$E_{max} = E(\mathbf{R}) = E_0 + 6\gamma$$
$$E_{min} = E(\mathbf{\Gamma}) = E_0 - 6\gamma$$

2) $R\Gamma$ : $\frac{\pi}{a}(111) \rightarrow \frac{\pi}{a}(000)$;

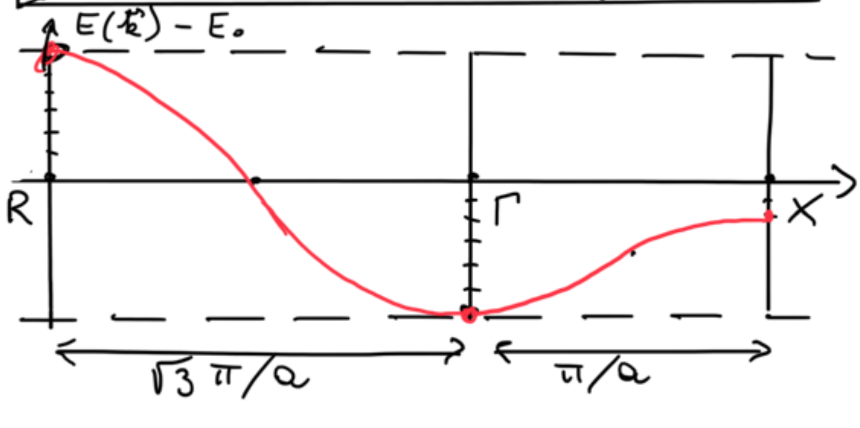
$\vec{k} \in R\Gamma$ : $\vec{k} = \frac{\pi}{a}(111)\xi$ con $0 \le \xi \le 1$

$$\boxed{E(\vec{k} \in R\Gamma) = E_0 - 6\gamma \cos \pi\xi}$$

$\Gamma X$ : $(000) \rightarrow \frac{\pi}{a}(100)$;

$\vec{k} \in \Gamma X$ : $\vec{k} = \frac{\pi}{a}(100)\nu$ con $0 \le \nu \le 1$

$$\boxed{E(\vec{k} \in \Gamma X) = E_0 - 4\gamma - 2\gamma \cos \pi\nu} \rightarrow E(\mathbf{X}) = E_0 - 2\gamma$$



3) p.ti a sella?

Devono essere p.ti stazionari: $\vec{\nabla}_k \mathcal{E} = 0 \Rightarrow$

$$\vec{\nabla}_k \mathcal{E} = 2\gamma a\,(\operatorname{sen} k_x a, \operatorname{sen} k_y a, \operatorname{sen} k_z a) = 0 \Rightarrow$$

$$k_\alpha = m_\alpha \pi/a$$

$$\frac{\partial^2 \mathcal{E}}{\partial k_\alpha \partial k_\beta} = \delta_{\alpha\beta}(-2\gamma a^2)\cos k_\alpha a \Rightarrow$$

$$\left.\frac{\partial^2 \mathcal{E}}{\partial k_\alpha \partial k_\beta}\right|_{\substack{\text{p.ti} \\ \text{stazionari}}} = -2\gamma a^2 \delta_{\alpha\beta} \cos m_\alpha \pi$$

Poiché nei p.ti a sella le derivate seconde hanno segno diverso in due diverse direz., si vede subito che questo succede ad es. per $m_1 = \pm 1$, $m_2 = m_3 = 0$ e simili, cioè:

$$\boxed{X = \frac{\pi}{a}(100) \text{ e } M = \frac{\pi}{a}(110) \text{ sono p.ti a sella}}$$

4) DOS attorno a $E_{min}$?

$$g(\mathcal{E}) = \frac{1}{4\pi^3}\int_{\mathcal{E}\text{ cost.}} \frac{dS}{|\vec{\nabla}\mathcal{E}|} = ?$$

Sviluppo $\mathcal{E}(k)$ attorno a $\Gamma = (000)$ (min.):

$$\mathcal{E}(k) \cong E_0 - 2\gamma\left[3 - \left(\frac{ak_x}{2}\right)^2 - \left(\frac{ak_y}{2}\right)^2 - \left(\frac{ak_z}{2}\right)^2\right]$$

$$\boxed{\mathcal{E}(k) \cong E_0 - 6\gamma + \gamma a^2 k^2}$$

da confrontare con la solita espressione con la massa efficace:

$$\mathcal{E}(k) \cong E_{min} + \frac{\hbar^2 k^2}{2m^*} \; : \; \begin{cases} E_{min} = E_0 - 6\gamma \\ \quad\;\;\, = E(\Gamma) \\ \dfrac{\hbar^2}{2m^*} = \gamma a^2 \end{cases}$$

$$m^* = \frac{\hbar^2}{2\gamma a^2}$$

L'espressione per gli $e^-$ liberi:

$$\boxed{g(\mathcal{E}) = \frac{m}{\hbar^2 \pi^2}\sqrt{\frac{2m\mathcal{E}}{\hbar^2}}\,, \quad \mathcal{E}>0}$$ (A&M 2.61)

può essere qui usata, con $\begin{cases} \mathcal{E} \to \mathcal{E} - E_{min} \\ m \to m^* \end{cases}$

5) Somme di Bloch in $\mathbf{\Gamma}$ e $\mathbf{R}$:

$$\psi_{\vec{k}}(\vec{r}) = \sum_{\vec{R}} e^{i\vec{k}\cdot\vec{R}} \phi_{1s}(\vec{r}-\vec{R}), \quad \text{con } \vec{R} = \sum_i n_i \vec{a}_i = (n_1, n_2, n_3)a$$

$$\psi_{\Gamma}(\vec{r}) = \sum_{\vec{R}} \phi_{1s}(\vec{r}-\vec{R})$$ (stessa fase su tutti i siti atomici)

$$\psi_{\mathbf{R}}(\vec{r}) = \sum_{n_i} (-1)^{n_1+n_2+n_3} \phi_{1s}(\vec{r}-(n_1, n_2, n_3)a)$$

(a scacchiera)

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